The GEANT Low Energy Compton Scattering (GLECS) Package for use in Simulating Advanced Compton Telescopes

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Abstract

Compton gamma-ray imaging is inherently based on the assumption of gamma rays scattering with free electrons. In reality, the non-zero momentum of target electrons bound in atoms blurs this ideal scattering response in a process known as Doppler broadening. The design and understanding of advanced Compton telescopes thus depends critically on the ability to accurately account for Doppler broadening effects. For this purpose, a Monte Carlo package that simulates detailed Doppler broadening has been developed for use with the powerful, general-purpose GEANT3 and GEANT4 radiation transport codes. This paper describes the design of this package, and illustrates results of comparison with selected experimental data.

Key words: Compton scattering, computer modeling and simulation, Monte Carlo method, gamma-ray telescopes
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1 Introduction

As modern instruments for high-energy astronomy become increasingly complex, the need for computer simulation tools for investigating instrument design and performance becomes ever more crucial. Advanced Compton telescopes for use in MeV gamma-ray astronomy are a particular challenge to instrument developers. Not only are the instruments, themselves exceedingly complex — with thousands or even millions of detector elements — but they also need to operate effectively in an exceedingly complicated, background-dominated environment. Monte Carlo radiation transport simulations offer a

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practical means to meet many of the challenges involved in designing, developing, and operating these instruments. To be effective, however, the simulations must accurately reflect the underlying particle interaction physics, the details of the instrument and electronics, and the incident source/background particle distributions.

Fortunately, the high-energy nuclear and particle physics communities have faced similar problems for decades, and as a result developed several powerful, general-purpose simulation packages. Among the most effective and widely used of these packages are the "Geometry and Tracking" (GEANT) codes developed principally at CERN. In both its FORTRAN (GEANT3; Apostolakis et al. 1993) and C++ (GEANT4; Agostinelli et al. 2003) incarnations, GEANT provides facilities for modeling complex instrument geometry, composition, and operating parameters within the context of a substantial range of particle interaction physics. There is, however, one significant inadequacy in these codes with respect to Compton instruments: neither GEANT3 nor GEANT4 include the detailed physics of Compton scattering in the low-energy regime where atomic binding effects become important. To address this shortcoming I developed the GEANT Low-Energy Compton Scattering (GLECS) codes that augment GEANT's Compton scattering physics capabilities in this area that is crucial for designing and understanding advanced Compton telescopes. The remainder of this paper describes the low-energy Compton scattering problem, and how it is addressed in the GLECS package.

2 Compton Scattering with Bound Atomic Electrons

For convenience and practicality, most general-purpose Monte Carlo packages like GEANT treat Compton scattering in the limit where the target electron is at rest in free space. In this limiting case, conservation of energy and momentum leads to the famous Compton formula:

$$k_{\mathrm{free}} = \frac{k_{\mathrm{o}}}{1 + \frac{k_{\mathrm{o}}}{m_{\mathrm{o}}c^2}(1 - \cos\varphi)} \ , \tag{1}$$

where k_{o} is the incident photon energy, k_{free} is the scattered photon energy (in the free-electron limit), φ is the polar photon scatter angle, and $m_{\mathrm{o}}c^2$ is the electron rest energy. This formula unambiguously relates the scatter angle to the incident and scattered photon energies, thereby forming the fundamental basis of the Compton imaging technique.

In real detectors, target electrons are neither free, nor at rest — they are bound to their atomic nuclei with non-zero orbital momentum. In this case, the analog to the Compton formula can be approximated as (Ribberfors, 1975):

$$k = k_{\mathrm{free}} \left(1 - \frac{p_{\mathrm{z}} |\boldsymbol{k_{\mathrm{o}}} - \boldsymbol{k}|}{m_{\mathrm{o}} c \; k_{\mathrm{o}}} \right), \tag{2}$$

where k is the scattered photon energy and p_{z} is the component of the pre-collision electron's orbital momentum in the direction of the incident photon. Because p_{z} depends on the quantum mechanical state of the electron orbit, it can only be constrained in a statistical sense. There is thus no unique value of k for a particular set of $(k_{\mathrm{o}}, \varphi)$. Rather, the scattered photon energy is blurred about the value of k_{free} in an effect known as "Doppler broadening." The amount of broadening depends on the target electron's atomic shell state (inner shells having larger p_{z} result in greater broadening), the photon scatter angle (large scatter angles being affected more than small scatter angles), and the incident photon energy (the magnitude of Doppler broadening decreasing as $\sim 1/k_{\mathrm{o}}$). Atomic binding also introduces a scattering form factor that has the effect of suppressing the free-electron Klein-Nishina cross section for forward scattering at lower energies.

For many practical purposes, such as modeling bulk spectrometers, the effects of atomic binding on Compton scattering are insignificant. These effects do, however, place a firm physical limit on the angular resolution achievable with Compton imaging. As advanced Compton telescope designs employ component detectors with increasingly better energy and spatial resolution, the Doppler limit is quickly becoming the most significant limiting factor of the Compton imaging technique. It is thus crucial that simulation tools for modeling Compton telescopes accurately account for these effects.

3 The GEANT Low-Energy Compton Scattering Package

All of the detailed physics of Compton scattering in the low-energy regime where bound electron effects are important have been incorporated into the GLECS [1] package. Versions of this package have been integrated into both GEANT3 (GLECS) and GEANT4 (G4LECS). The physics implementation algorithms are based on the work of Namito, Ban, and Hirayama (1994). This treatment accounts for bound electron effects in the "impulse approximation," where interactions between electron sub shells are ignored. The important implementation details include:

(A) The probability of a Compton scatter for a particular element is randomly sampled from total Compton cross sections obtained by interpolating Evalu-

[1] Publicly available at `http://nis-www.lanl.gov/~mkippen/actsim/`

ated Photon Data Library tables (EPDL97; Cullen, Hubbell, and Kissel 1997). These data include electron binding effects averaged over all atomic electron states, and are valid from ∼250 eV to 100 GeV. For compound materials, a weighted average of the elemental component cross sections is used, based on the relative number of electrons for each component element.

(B) The photon scatter angle φ for a particular element is randomly sampled from the differential Klein-Nishina cross section multiplied by the incoherent scattering form factor interpolated from EPDL97 data. The EPDL form factors represent the weighted average over all electron shells for particular element, and are valid over the same energy range as the total cross sections. For compound materials, a specific element is randomly sampled based on the relative number of electrons for each component element.

(C) The "Doppler broadened" scattered photon energy k is computed with Equation 2 using tabulated distributions of p_{z}. These distributions (known as "Compton profiles") for each atomic electron sub-shell are based on the Hartee-Fock calculations of Biggs, Mendelsohn, and Mann (1975). The appropriate sub-shell is first randomly sampled based on the electron occupancy per shell, then p_{z} is sampled from the appropriate sub-shell Compton profile. This allows the energies of the scattered photon and (by conservation of energy) scattered electron to be computed.

For consistency, and to repair low-energy failings of the standard GEANT algorithms, the GLECS packages also include detailed treatment of Rayleigh (i.e., coherent) scattering. In this treatment, total cross sections and coherent scattering form factors are based on interpolated EPDL97 data, similar to the treatment of Compton scattering.

4 Code Verification

As a verification, the GLECS codes were used to simulate the X-ray scattering experiments described in Namito et al. (1995). In these experiments, a collimated monochromatic beam of polarized 40-keV photons was scattered from various thin target disks, and then measured with two small germanium detectors oriented perpendicular to the beam. In the GLECS simulations, this setup was approximated by a conical shell target and a 2π annular detector ring that yield much greater computing efficiency for unpolarized photons.

Results for targets made of lead (0.5-mm thick), copper (2.0-mm thick), and carbon (0.589-mm thick) are illustrated in Figure 1. Each case includes 10,000 simulated germanium deposition events using G4LECS and the G4LowEnergy Compton code that was included in GEANT4.4.1 (this code does not in-

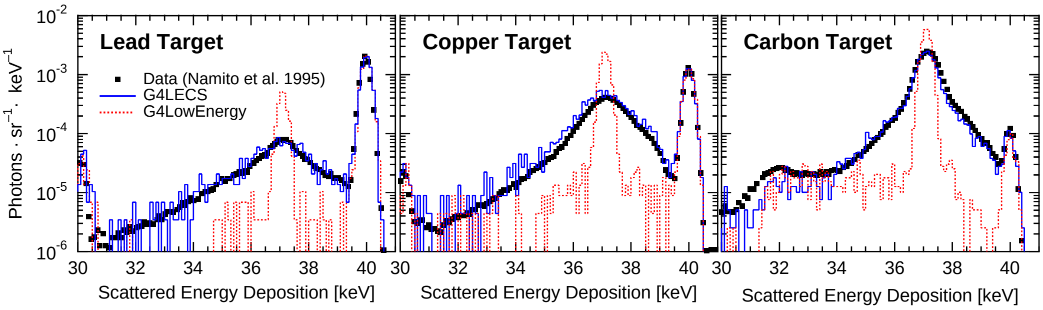

Fig. 1. Comparison of GLECS simulations and experimental data.

clude Doppler broadening). All other physical effects are included using the G4LowEnergy classes. The raw simulation data have been histogramed and broadened by a Gaussian smearing function that corresponds to the reported resolution of the germanium detectors (0.35 keV FWHM), and the peak histogram values normalized to the experimental data.

The peak at 40 keV in each test corresponds to Rayleigh-scattered photons that loose no energy in the interaction, and thus deposit their full energy in the germanium. The peak near 37 keV corresponds to the most likely energy of a 90 deg Compton scattered photon (i.e., k_{free}). In the case of copper and lead, there are additional X-ray escape features near 30 keV. In the case of carbon, there is a feature near 32 keV due to multiply scattered photons.

There is reasonably good agreement between the data and the G4LECS simulations. The small differences that do exist are probably due to statistical fluctuations, differences between the simulation and experimental geometries, or the fact that the simulations do not include a polarized beam. Comparison between the G4LECS and G4LowEnergy results dramatically illustrate the effects of Doppler broadening, which causes a significant spread in the Compton-scattered photon energies that increases with the Z of the target material. The approximate FWHM of the scattered photon energy distributions are 1.2 keV, 1.5 keV, and 1.8 keV for C, Cu, and Pb, respectively — much larger than the germanium detector resolution. Similar results were obtained using the GEANT3 version of GLECS.

5 Conclusion

The test results presented in this paper indicate that the GLECS codes do a reasonably accurate job of simulating Compton scattering in the low-energy regime. With GLECS, the power and flexibility of GEANT may now be applied to the difficult tasks of designing and modeling advanced Compton telescopes. While for some applications or instrument designs the details of low-energy scattering physics may be essentially irrelevant, these effects are important for most of the advanced telescope concepts that use high-resolution component detectors. For example, Zoglauer and Kanbach (2003) used GLECS to simulate a wide range of scattering materials and found the Doppler limiting angular resolution to be a significant factor for all practical detector materials.

Although the GLECS codes do introduce some added computing overhead, the performance is within $\sim$5% of that using standard GEANT3/4 Compton physics algorithms, which should not be a significant burden to users. A key planned future enhancement is to include the effects of polarized photons.

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